Reaction mechanisms and kinetics of processing glucose, xylose and glucose-xylose mixtures under hot compressed water conditions for predicting bio-crude composition

Grigoras, Ionela; Toor, Saqib Sohail; Rosendahl, Lasse Aistrup

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Reaction mechanisms and kinetics of processing glucose, xylose and glucose-xylose mixtures under hot compressed water conditions for predicting bio-crude composition

Ionela F. Grigoras, Saqib S. Toor, Lasse A. Rosendahl*

Aalborg University, Department of Energy Technology, Pontoppidanstræde 101, 9220 Aalborg, Denmark

**ifg@et.aau.dk*

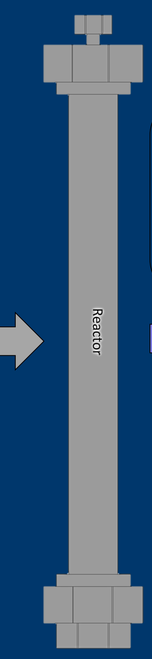
Mechanisms for bio-crude formation during the conversion of glucose, xylose and glucose-xylose mixtures as biomass model compounds under hot compressed water conditions are investigated. Studies in literature have shown that the diverse products formed at the early stages of glucose or xylose conversion are 5-HMF, erythrose, glyceraldehyde, dihydroxyacetone, pyruvaldehyde, and saccharinic acids resulted through reactions such as dehydration, retro-aldol condensation and isomerization. However, these compounds are mostly water soluble compounds and lack the final steps towards formation of water insoluble components at longer reaction times. The effects of pressure, pH, catalyst and reaction time on the main products are examined thoroughly. The possible routes for the formation of oil compounds are developed.

HTL process

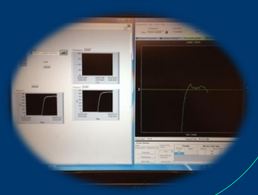
Glucose

Xylose

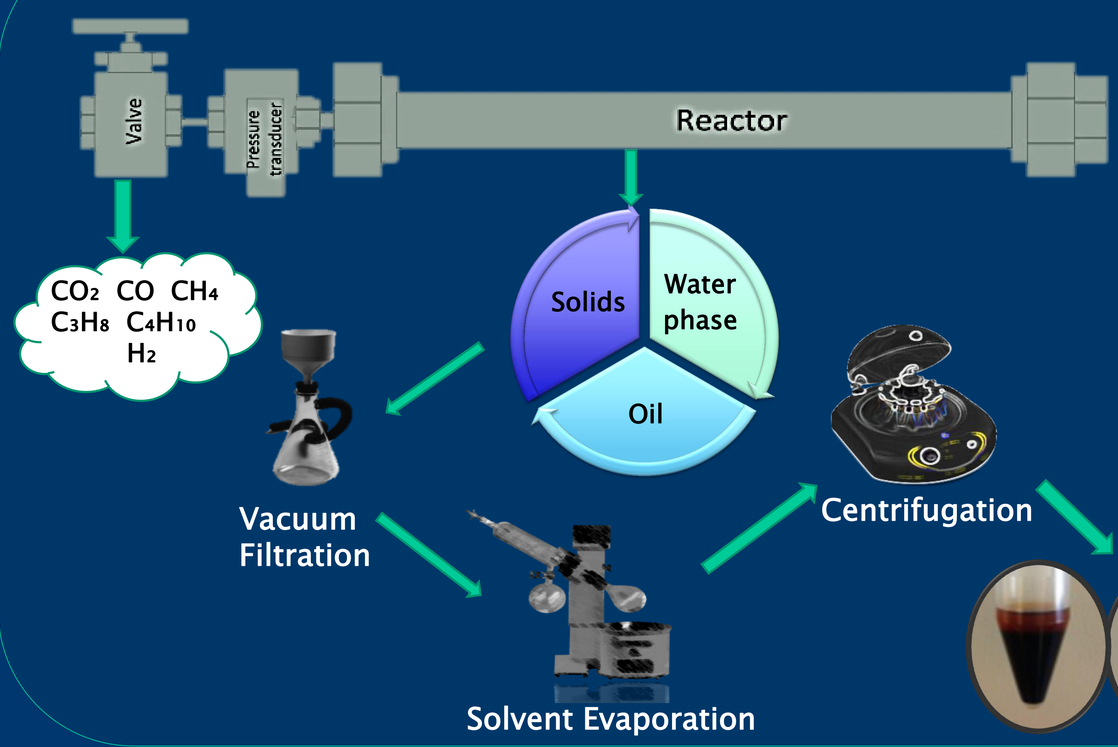
Mixture of Glucose – Xylose



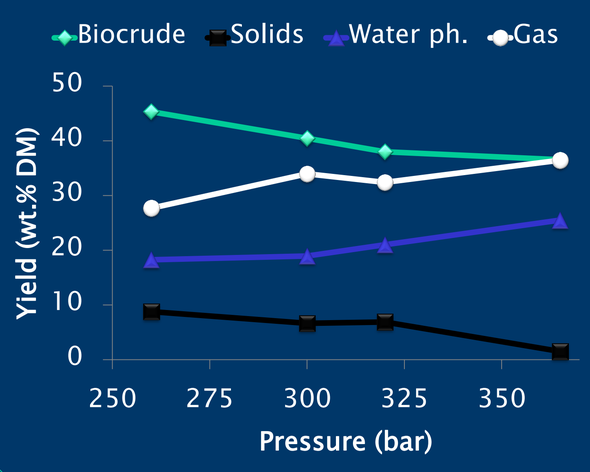
400 ° C
250 – 350 bar
0 – 20 min
0 – 4 % catalyst

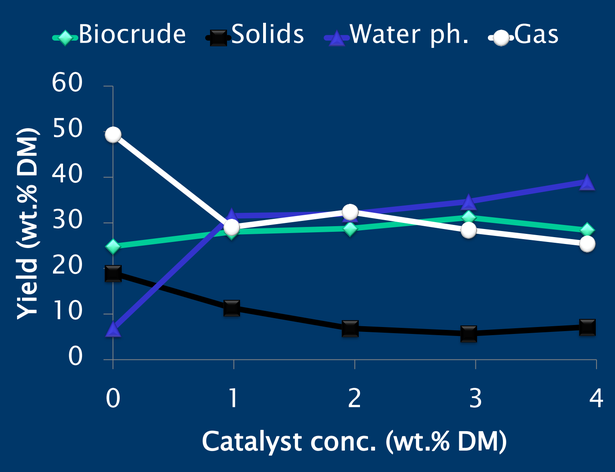


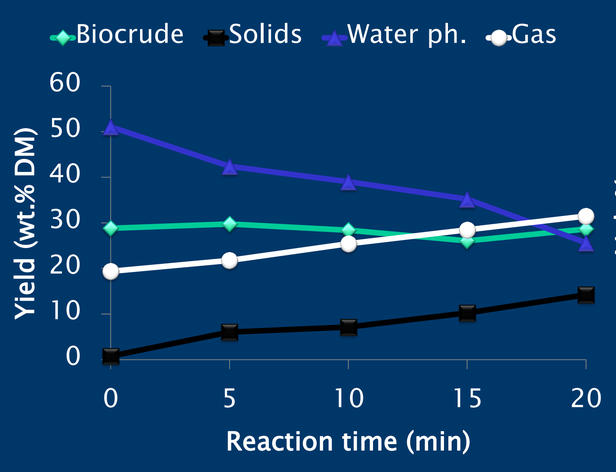
Separation process

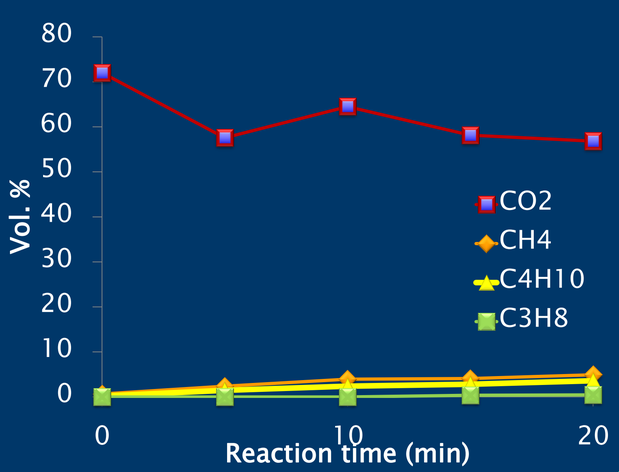


Parametric study – Glucose case

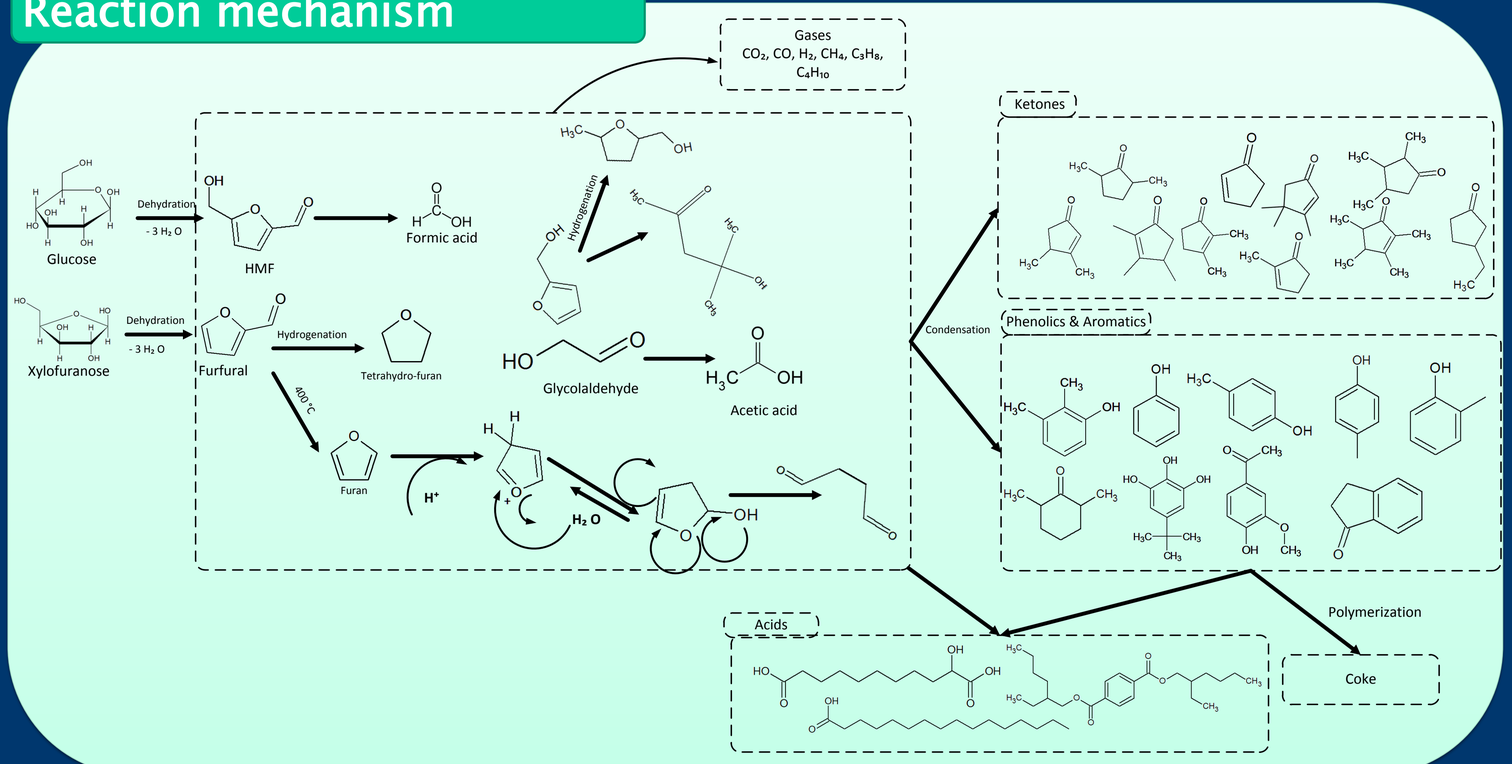








Reaction mechanism



Conclusions

- Pressure and reaction time did not influence the final pH of the product significantly; Catalyst concentration was found to be the only factor affecting the final pH of the product.
- **Reaction time** influences gas composition; longer reaction time increased the concentration of CH_4, C_3H_8 and C_4H_{10} in the gas phase, whereas the CO_2 decreased for glucose and mixtures of glucose-xylose, but increased in the case of xylose.
- At **short reaction times** furan based compounds such as furfurals, furanones, tetrahydrofuranols will be kept in the biocrude composition. At **longer reaction times**, the furan ring opens under the water attack. The ring opening leads to production of ketones and aldehydes. Analysis of water soluble products and biocrude showed a decrease in the furan-methanol concentration as the reaction time was increased during the HTLprocess. At the same time, the concentration of 4-hydroxy-4-methyl-2-pentanone increased. Long reaction times also favor formation of carboxylic acids.

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